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ORTHOGONAL POLYNOMIALS IN ANALYTICAL METHOD OF SOLVING DIFFERENTIAL EQUATIONS DESCRIBING DYNAMICS OF MULTILEVEL SYSTEMS*

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Abstract

An effective method to obtain exact analytical solutions of equations describing the coherent dynamics of multilevel systems is presented. The method is based on the usage of orthogonal polynomials, integral transforms and their discrete analogues. All the obtained solutions are expressed by way of special or elementary functions.

Key words: integral transforms, orthogonal polynomials, multilevel quantum systems.

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1 INTRODUCTION

Orthogonal polynomials and functions are used as the complete bases of the solutions of differential and difference equations. In quantum physics they are of primary importance in the construction of wave functions which are orthogonal by definition. In present paper orthogonal polynomials and functions are used to describe excitation of quantum multilevel systems in high-power laser field.

The Schrödinger equation for a multilevel system being exciting in a monochromatic laser field looks like

$$-ida_n(t)/dt = f_{n+1}\exp\left(-i\varepsilon_{n+1}t\right)\,a_{n+1}(t) + f_n\exp\left(i\varepsilon_n t\right)\,a_{n-1}(t), \quad n = 0, 1, 2, \ldots \tag{1}$$

where f_n is a dipole moment function for the transitions $n{-}1 \leftrightarrow n$ (that is $\mu_{n-1,n} = f_n\mu_{0,1}$), ε_n is a frequency detuning. Probability amplitudes $a_n(t)$ allow to determine levels populations $\rho_n(t) = |a_n(t)|^2$, an average number of absorbed photons $< n >= \sum_{n=1}^{n_{max}} n\rho_n(t)$ etc.

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To obtain the solution of (1) we introduce an analytical method [1] based on orthogonal functions $p_n(z)$.

2 FROM ORTHOGONAL POLYNOMIALS TO QUANTUM SYSTEMS

We seek the solution of (1) in form

$$a_n(t) = \int_A^B \sigma(x) \frac{p_0(x)}{d_0} \frac{p_n(x)}{d_n} \exp\left[it\left(r\theta(x) + s_n\right)\right] dx, \tag{2}$$

where d_n is the squared norm and s_n determines the frequency detuning: $\varepsilon_n = s_n - s_{n-1}$.

At $t = 0$ the solution (2) passes into the orthogonality relation for the functions $p_n(x)$. Hence we obtain the initial condition for Eq. (1): $a_n(t) = \delta_{n,0}$. The functions $p_n(x)$ should satisfy the recurrence relation

$$\left(r\theta(x) + s_n\right) \frac{p_n(x)}{d_n} = f_n \frac{p_{n-1}(x)}{d_{n-1}} + f_{n+1} \frac{p_{n+1}(x)}{d_{n+1}}. \tag{3}$$

Initially we select the sequence of orthogonal functions which determines the quantum system to be investigated. The takeoff criterion is the relevant recurrence relation which allows to find both the constant r and the functions f_n and s_n. After that we obtain the analytical solution of (1) using the integral transform like (2).

The application of analytical method (1–3) makes possible describing dynamics of manifold quantum models including: N-level and infinite-level, equidistant and non-equidistant, excited resonantly and nonresonantly, closed and nonclosed, excited by monochromatic field and laser pulse. Gegenbauer, Jacobi, Pollaczek, Laguerre, Meixner, Krawtchouk, Hahn polynomials; Szegö-Jacobi polynomials built using the Szegö method; Christoffel-Legendre orthogonal polynomials built by using the Christoffel formula; orthogonal Gauss hypergeometric functions are used by us to obtain the exact solutions for these systems.

This quantum systems manifold includes the systems with various characteristics, first of all with qualitatively different dipole moment functions f_n. In particular Jacobi, Legendre and Chebyshev of the 1$^{\text{st}}$ kind polynomials lead to the quantum systems with $f_n \leq 1$, Jacobi, Gegenbauer and Chebyshev of the 2$^{\text{nd}}$ kind polynomials — to the systems with $1 \leq f_n < \sqrt{n}$, Pollaczek, Laguerre and Meixner polynomials give rise to two sets of the systems with $\sqrt{n} < f_n \leq n$ and $f_n > n$. It is known that Hermite polynomials correspond to the harmonic oscillator ($f_n = \sqrt{n}$).

Thus the existing diversity of orthogonal polynomials makes possible to obtain the solutions of (1) describing the dynamics of various quantum systems with different properties. Each orthogonal polynomials sequence (OPS) can be put in unique correspondence with some quantum system. Below we shall discuss some examples.

3 JACOBI POLYNOMIALS

Let's consider the quantum systems which have been built by means of Jacobi polynomials. The dipole moment function following from a recurrence relation (3) looks like

$$
\begin{aligned}
f_n &= \frac{2r}{2n+\alpha+\beta}\left[\frac{n\,(n+\alpha)\,(n+\beta)\,(n+\alpha+\beta)}{(2n+\alpha+\beta-1)\,(2n+\alpha+\beta+1)}\right]^{1/2}, && (4)\\
r &= \frac{\alpha+\beta+2}{2}\left[\frac{\alpha+\beta+3}{(\alpha+1)\,(\beta+1)}\right]^{1/2}, \quad \alpha>-1,\ \beta>1. && (5)
\end{aligned}
$$

Thus the dipole moments of higher transitions tend to the constant value $r/2$. Energy levels of the Jacobi systems are nonequidistant but the frequency detuning decreases with n approximately as n^{-3}, i.e. the highest levels are practically equidistant and they are being excited resonantly.

Jacobi OPS contains two parameters α and β which determine the energy levels positions. Therefore we obtain two-parameter continual family of multilevel quantum systems. Each pair of (α,β) corresponds to the specific Jacobi quantum system which is described by dipole moment f_n and frequency detuning ε_n functions.

The solution of (1) for the Jacobi systems dynamics is expressed through the Kummer hypergeometric functions:

$$
\begin{aligned}
a_n(t) = (2irt)^n \left[\frac{(\alpha+1)_n\,(\beta+1)_n}{(\alpha+\beta+2)_{2n}\,(n+\alpha+\beta+1)_n\, n!}\right]^{1/2} \times \\
e^{it(r+s_n)}{}_1F_1\left(n+\alpha+1; 2n+\alpha+\beta+2; -2irt\right).
\end{aligned} \qquad (6)
$$

At $\alpha=\beta$ Jacobi polynomials $P^{(\alpha,\alpha)}(x)$ pass into Gegenbauer ones $C^{(\lambda)}(x)$, $\lambda=\alpha+1/2$. Thus Kummer function in (6) is reduced to a cylindrical function $J_{n+\lambda}(rt)$. The case $\alpha=\beta=1$ (Chebyshev polynomials of the 2^{nd} kind) gives so called equal-Rabi system $f_n\equiv 1$, for $\alpha=\beta=0$ (Chebyshev polynomials of the 1^{st} kind) we obtain the system with $f_1=1, f_n=1/\sqrt{2}$, $n\geq 2$. The levels of both Gegenbauer and Chebyshev systems are equidistant, the excitation is resonant.

An interesting situation arises in a case $\alpha=-\beta$ when

$$
f_n=\left[3\left(n^2-\alpha^2\right)/\left(1-\alpha^2\right)\left(4n^2-1\right)\right]^{1/2}, \quad s_n=\alpha\left[3/\left(1-\alpha^2\right)\right]^{1/2}\delta_{n,0}.
$$

Here the frequency detuning $\varepsilon_n=-s_0\delta_{n,1}$, the levels are equidistant everywhere except for the first transition and only this transition is nonresonant. In particular at $\alpha=-\beta=\pm 1/2$ we obtain $f_n\equiv 1$, $\varepsilon_n=-\delta_{n,1}$ and the expressions for levels populations $\rho_n(t)=|a_n(t)|^2$ reshape an especially simple form $\rho_n\left(t\right)=J_n^2\left(2t\right)+J_{n+1}^2\left(2t\right)$.

4 KRAWTCHOUK POLYNOMIALS

Using Krawtchouk polynomials of discrete variable [2] we can describe the nonresonant excitation of the quantum systems with finite number of equidistant levels and dipole moment function

$$f_n = \left[\frac{n\,(N-n+1)}{N}\right]^{1/2}, \qquad n = \overline{0,N}, \quad N = 1,2,\ldots. \tag{7}$$

The analytical solution of (7) is expressed [3] by way of elementary functions:

$$\begin{aligned} a_n(t) &= \left[\binom{N}{n} y^n(t)\right]^{1/2} \left\{[1-(1+\sigma)y(t)]^{1/2} + i\,[\sigma y(t)]^{1/2}\right\}^{N-n} \exp\left[it\varepsilon(n-N/2)\right]; & (8)\\ \rho_n(t) &= \binom{N}{n} y^n(t)\,[1-y(t)]^{N-n}; & (9)\\ < n > &= Ny(t) & (10) \end{aligned}$$

where

$$y\,(t) = \frac{\sin^2\left\{[(1+\sigma)\,/N]^{1/2}\,t\right\}}{(1+\sigma)}, \qquad \sigma = N\varepsilon^2/4. \tag{11}$$

The Krawtchouk systems are suitable exactly solvable models for vibrational excitation of a molecule in high-power infrared laser fields. The solution describes an excitation with arbitrary detuning of laser frequency from the system transitions frequency. The case $p = ^1/_2$ corresponds to the resonant excitation. Krawtchouk systems family includes both two-level and three-level systems and harmonic oscillator as special and limit cases ($N=1$, $N=2$ and $N\to\infty$ correspondingly).

Thus the Krawtchouk polynomials give a possibility to build one-parametric family of quantum multilevel systems and to obtain exact analytical solutions of the equations describing the excitation dynamics. The Krawtchouk systems family is an extensive class of multilevel models for various dynamical processes in spectroscopy, nonlinear optics and the other fields.

The method under consideration gives also the possibility of solving the equations which are more complicated then (1). Let the quantum system consist of finite number of degenerate levels. The equation describing the resonant excitation of such a system is

$$\begin{aligned} -i\frac{da_{n,m}(t)}{dt} &= \Omega\,[f_{n+1}a_{n+1,m}(t) + f_n a_{n-1,m}(t)] + \qquad (12)\\ &\Omega'\,[f_{n+1}g_{m+1}a_{n+1,m+1}(t) + f_{n+1}g_m a_{n+1,m-1}(t) + f_n g_{m+1}a_{n-1,m+1}(t) + f_n g_m a_{n-1,m-1}(t)] \end{aligned}$$

where Ω and Ω' are Rabi frequencies, $f_n = [n(N-n+1)/N]^{1/2}$ and $g_m = [m(M-m+1)/M]^{1/2}$ are dipole moment functions for the interlevel and intersublevel transitions correspondingly, $n = \overline{0,N}$, $m = \overline{0,M}$; $M, N = 1,2,\ldots$ Here we assume $a_{n,m}(0) = \delta_{n,0}\delta_{m,0}$ as an initial condition and $\Delta n = \pm 1$, $\Delta m = 0, \pm 1$ as the selection rules.

The solution of (12) is expressed via Krawtchouk polynomials and elementary functions:

$$a_{n,m} = \frac{i^n}{2^{M-m}}\left[\frac{\binom{N}{n}}{\binom{M}{m}}\right]^{1/2} \sum_{j=0}^{M} k_m^{(1/2)}(j,M)\binom{M}{j}\sin^n\tau_j\,\cos^{N-n}\tau_j \tag{13}$$

where $\tau_j = \left(t/\sqrt{N}\right)\left[\Omega + \Omega'(2j - M)\Big/\sqrt{M}\right]$.

Selecting other orthogonal polynomials we can obtain the solutions of Eq. (12) for different types of f_n and g_m.

5 CHRISTOFFEL-LEGENDRE POLYNOMIALS

Let's consider the solution of (1) using Christoffel-Legendre orthogonal polynomials [4]

$$p_n(x) = \frac{b}{b-x}\left[P_n(x) - \kappa_n^{-1}(b)P_{n+1}(x)\right], \qquad \kappa_n(b) = P_{n+1}(b)/P_n(b) \tag{14}$$

built with Christoffel formula [5] using Legendre polynomials $P_n(x)$. The polynomials $p_n(x)$ are orthogonal on an interval $[-1, 1]$ with respect to the weight

$$\sigma(x) = (b-x)/b, \qquad b \geq 1 \tag{15}$$

and squared norm

$$d_n = \left\{\,[2/\,(n+1)]\, b/\kappa_n\,(b)\right\}^{1/2} \tag{16}$$

They satisfy the recurrence relation (3) ($\theta(x) \equiv x$) where

$$\begin{aligned} f_n &= r\,(n/(2n+1))\,d_{n-1}/d_n, \\ r &= 3d_1/d_0, \\ s_n &= r\left(\frac{n+1}{2n+1}\kappa_n(b) - \frac{n+2}{2n+3}\kappa_{n+1}(b)\right). \end{aligned} \tag{17}$$

The application of Christoffel-Legendre polynomials in (2) gives [4] the analytical solution

$$a_n(t,b) = i^n\left(\frac{\pi}{2}\right)^{\frac{1}{2}}\frac{d_0}{d_n}\,\frac{\exp\left(is_n\,t\right)}{(r\,t)^{1/2}}\left[J_{n+0,5}\,(r\,t) - i\,\kappa_n^{-1}\,(b)\;J_{n+1,5}\,(r\,t)\right] \tag{18}$$

of (1). This solution describes the excitation of one-parameter family of multilevel Christoffel-Legendre systems with nonequidistant energy levels, i.e. $\varepsilon_n \neq$ const.

6 LEGENDRE FUNCTIONS OF THE FIRST KIND

Another quantum system can be built by using the functions

$$p_n^\lambda(x) \;=\; (-i)^\mu\Gamma(\mu+1)P_{-\lambda}^{-\lambda-\mu}(x)\Big|_{\mu=n}, \tag{19}$$

being a special case of Legendre function of the 1st kind $P_\nu^\mu(x)$. The functions $p_n^\lambda(x)$ satisfy the recurrence relation (3) where

$$\begin{aligned} f_n &= \left|\frac{n\,(2\lambda+n-1)\;(\lambda+1)}{2(\lambda+n-1)\,(\lambda+n)}\right|^{1/2}, \qquad s_n \equiv 0, \\ r &= i\sqrt{2\,|\lambda+1|}, \qquad \theta(x) = \frac{x}{\sqrt{x^2-1}}, \end{aligned} \tag{20}$$

and

$$d_n = \left|\Gamma(1-2\lambda-n)\Gamma(n+1)\,/(\lambda+n)\right|^{1/2}, \quad \lambda<-1, \quad 0\le n\le|\lambda|\,. \tag{21}$$

For $p_n^\lambda(x)$ is correct

$$p_n^\lambda(x) \;=\; 2^\lambda i^n\,\frac{\Gamma\,(-2\lambda-n+1)n!}{\Gamma\,(-\lambda+1)}\left(x^2-1\right)^{-\lambda/2}C_n^\lambda\left(\frac{x}{\sqrt{x^2-1}}\right), \quad \lambda<-1, \quad 0\le n\le\;|\lambda| \tag{22}$$

where C_n^λ are Gegenbauer functions [6] of a complex argument z

$$C_\alpha^\lambda(z)=\frac{\Gamma(\alpha+2\lambda)}{\Gamma(\alpha+1)\Gamma(2\lambda)}\,{}_2F_1\left(\begin{matrix}-\alpha,\;\alpha+2\lambda\\ \lambda+1/2\end{matrix}\,\middle|\,\frac{1-z}{2}\right). \tag{23}$$

Functions p_n^λ are orthogonal on the discrete interval:

$$\sum_{l=0}^{N-1}\sigma^{(N)}(x_l)p_m^\lambda(x_l)p_n^\lambda(x_l)=\delta_{m,n}d_n^2, \quad N>|1-\lambda|\,, \quad \lambda<-1 \tag{24}$$

with respect to the weight function

$$\sigma^{(N)}(x_l)=\frac{\mathcal{K}_N}{\mathcal{K}_{N-1}}\left(\frac{2^{-\lambda}\Gamma(1-\lambda)d_{N-1}}{\Gamma(N)\Gamma(2-2\lambda-N)}\right)^2\left(x_l^2-1\right)^\lambda\left(C_{N-1}^\lambda(z_l)\frac{d}{d\,z_l}C_N^\lambda(z_l)\Big|_{z_l=x_l\big/\sqrt{x_l^2-1}}\right)^{-1} \tag{25}$$

where z_l are the roots of a polynomial of degree N, $C_N^\lambda(z_l)=0, x_l=z_l/\sqrt{z_l^2-1}$ and $\mathcal{K}_N$ is the higher coefficient of this polynomial. Thus the solution of (1) for the system of N equidistant levels in a resonant field (at $f_N\equiv 0$ and $\varepsilon_n\equiv 0$) looks like

$$a_n^{(N)}(t)=\sum_{l=0}^{N-1}\sigma^{(N)}(x_l)\left(\frac{p_m^\lambda(x_l)}{d_m}\right)^*\frac{p_n^\lambda(x_l)}{d_n}\exp\left[\frac{itr\,x_l}{\sqrt{x_l^2-1}}\right]. \tag{26}$$

7 FROM QUANTUM SYSTEMS TO ORTHOGONAL POLYNOMIALS

Previously we initially selected orthogonal functions to obtain the solution of the equation (1) for qualitatively and quantitatively different quantum systems. Having done so we get the compact solutions which are expressed via known special or even elementary functions. When OPS contains the parameters the solution describes the dynamics of continual or discrete family of quantum systems. From the other side the imperfection of this method is that it is not always possible to obtain exact analytical solutions for a target system with the given dipole moments function f_n.

Let's consider the quantum system with an arbitrary dipole moments function being restricted with the case of resonant excitation and a finite number of equidistant levels. Now (1) reduces to the system of $N+1$ uniform linear differential equations

$$\begin{aligned}
-\,i\;da_0(t)/dt &= f_1a_1(t);\\
-i\;da_n(t)/dt &= f_{n+1}a_{n+1}(t)+f_na_{n-1}(t); \quad n=\overline{1,N-1}\\
-i\;da_N(t)/dt &= f_Na_{N-1}(t)
\end{aligned} \tag{27}$$

(some special cases of f_n have been studied in [7]).

Let us seek the solution of (27) in the form

$$a_n(t) = \sum_{k=0}^{N} \sigma_k p_n(\Lambda_k) \exp(i\Lambda_k t) \tag{28}$$

where p_n, Λ_k and σ_k are the functions to be determined. Substituting (28) into (27) we come to a three-term recurrence relation for p_n:

$$f_{n+1} p_{n+1}(\Lambda_k) + f_n p_{n-1}(\Lambda_k) = \Lambda_k p_n(\Lambda_k), \quad p_{-1} = 0, \quad p_0 = \mathrm{const} \tag{29}$$

Therefore p_n are the polynomials orthogonal with respect to variable Λ_k (generally on a nonuniform grid).

This truncated orthogonal polynomials $p_n(\Lambda_k)$ differ from the common polynomials listed above which satisfy the same dipole moment function f_n with an interval of n change. Let's discover the basic characteristics of these polynomials.

It is known that the recurrence relation like (3) determines an orthogonal polynomial up to an arbitrary constant factor. The comparison of (3) and (29) shows that the polynomials $p_n(\Lambda_k)$ are orthonormalized. Therefore it is natural to choose the normalization $p_0(\Lambda_k) \equiv 1$.

Suppose that initially all the particles are concentrated on the lower level, in other words $a_n(0) = \delta_{n,0}$. Then it follows from (28) that

$$\sum_{k=0}^{N} \sigma_k p_n(\Lambda_k) p_0(\Lambda_k) = \delta_{n,0}. \tag{30}$$

Thus the integration constants σ_k are the weight coefficients of polynomials p_n with respect to the variable Λ_k.

To determine Λ_k we shall use the last equation of (27); it gives

$$f_N p_{N-1}(\Lambda_k) = \Lambda_k p_N(\Lambda_k). \tag{31}$$

Comparing (31) and (29) it is possible to conclude that Λ_k are the roots of the polynomial $p_{N+1}(\Lambda_k)$.

Calculation of the polynomials $p_n(\Lambda_k)$ by the recurrence relation (29) and determination of weight coefficients σ_k from the system (30) are possible for any values of N. At the same time (30) is reduced eventually to the solving in radicals of the polynomial equations of the degree $N+1$. Generally it is possible only for $N+1 \leq 4$. However in the case of a resonant excitation the polynomials p_n contain only even or odd degrees of an argument (depending on n parity). Thus the roots of the polynomials up to the ninth degree can be always found analytically. However using some computer algebra system (e.g. `Mathematica`) it is possible to obtain the roots for the polynomials of higher degrees for some simple f_n. In any case it is possible to find these roots numerically with an arbitrary precision.

The method allows to obtain the solutions describing the dynamics of the quantum systems with an arbitrary dipole moment dependence on level number. When the solution of (1) with the same f_n but for infinite number of levels can be received under the formula (2) by selecting the relevant orthogonal polynomials it is interesting to compare the truncated polynomials with the common ones. From the comparison of (3) and Eq. (29) it follows that

$$p_n\left(\Lambda_k\right) = p_n^{(c)}\left(\Lambda_k/r\right) \tag{32}$$

where $p_n^{(c)}$ are common polynomials, $r = b_0 d_0/d_1$ [5], d_n is a squared norm, b_0 is defined from the recurrence relations for unnormalized polynomials: $p_{n+1}(x) + b_n p_{n-1}(x) = (rx + s_n)\, p_n(x)$. In particular if $R_k^{(N+1)}$ is the k^{th} root of $p_{N+1}^{(c)}$ then $\Lambda_k = rR_k^{(N+1)}$.

Methods (1–3) and (28) can be generalized to the system excitation in an arbitrary laser field, to the account of non-adjacent dipole transitions and for the systems of degenerate levels.

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